

# ORGANOMETALLICS

Supporting information for *Organometallics*, **1990**, 9(11), 2865 – 2867, DOI: [10.1021/om00161a008](https://doi.org/10.1021/om00161a008)

# SITA

# 2865-2867

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Table I. Atomic Coordinates for Nonhydrogen Atoms in  
Crystalline  $[\text{Sn}(\text{C}_6\text{H}_3(\text{C}_2\text{H}_5)_2)]_8^a$ 

Atom Type <sup>b</sup>	Fractional Coordinates			Equivalent Isotropic Thermal Parameter, B, $\text{\AA}^2 \times 10^3$ <sup>c</sup>
	$10^4 x$	$10^4 y$	$10^4 z$	
Sn <sub>1</sub>	505(1)	-594(1)	2106(1)	44(1)
Sn <sub>2</sub>	511(1)	-2778(1)	2118(1)	43(1)
Sn <sub>3</sub>	-649(1)	-2752(1)	1692(1)	42(1)
Sn <sub>4</sub>	-657(1)	-582(1)	1698(1)	43(1)
C <sub>1a</sub>	1009(7)	439(14)	1881(7)	59(7)
C <sub>1b</sub>	803(7)	1342(15)	1560(8)	81(9)
C <sub>1c</sub>	1145(8)	2058(14)	1462(9)	85(10)
C <sub>1d</sub>	1670(8)	1809(17)	1642(10)	99(11)
C <sub>1e</sub>	1886(8)	871(18)	1918(10)	105(12)
C <sub>1f</sub>	1566(8)	188(17)	2054(10)	81(10)
C <sub>1g</sub>	187(10)	1706(19)	1375(12)	97(14)
C <sub>1h</sub>	101(9)	2124(16)	1887(11)	115(13)
C <sub>1i</sub>	1840(7)	-820(16)	2361(10)	116(12)
C <sub>1j</sub>	1975(10)	-1586(18)	1989(12)	134(15)
C <sub>2a</sub>	912(6)	-3704(12)	1697(7)	45(6)
C <sub>2b</sub>	824(8)	-3517(17)	1140(8)	74(9)
C <sub>2c</sub>	1081(10)	-4043(20)	849(10)	111(13)
C <sub>2d</sub>	1390(10)	-4861(20)	1148(10)	112(13)
C <sub>2e</sub>	1503(8)	-5082(20)	1724(10)	93(10)
C <sub>2f</sub>	1241(7)	-4547(13)	2007(8)	68(8)
C <sub>2g</sub>	452(10)	-2628(18)	761(8)	117(13)
C <sub>2h</sub>	254(12)	-2601(28)	143(12)	184(17)

Table I. (continued)

Atom Type <sup>b</sup>	Fractional Coordinates			Equivalent Isotropic Thermal Parameter, B, Å <sup>2</sup> x 10 <sup>c</sup>
	10 <sup>4</sup> x	10 <sup>4</sup> y	10 <sup>4</sup> z	
C <sub>2i</sub>	1323(11)	-4886(17)	2619(9)	119(12)
C <sub>2j</sub>	1296(20)	-5697(22)	2806(15)	229(28)
C <sub>3a</sub>	-1295(6)	-3702(11)	1047(6)	44(5)
C <sub>3b</sub>	-1831(7)	-3539(14)	972(8)	70(7)
C <sub>3c</sub>	-2231(10)	-4196(18)	611(10)	96(11)
C <sub>3d</sub>	-2140(10)	-4929(20)	305(9)	98(11)
C <sub>3e</sub>	-1641(10)	-5105(16)	355(9)	92(11)
C <sub>3f</sub>	-1206(7)	-4446(15)	734(8)	69(8)
C <sub>3g</sub>	-2011(7)	-2703(15)	1288(9)	87(10)
C <sub>3h</sub>	-2330(10)	-1845(17)	896(10)	129(12)
C <sub>3i</sub>	-624(9)	-4706(17)	803(10)	128(14)
C <sub>3j</sub>	-320(11)	-5500(19)	1174(19)	194(23)
C <sub>4a</sub>	-1149(6)	391(12)	924(7)	58(6)
C <sub>4b</sub>	-1455(6)	1208(14)	982(10)	70(7)
C <sub>4c</sub>	-1713(7)	1861(16)	514(11)	88(10)
C <sub>4d</sub>	-1682(8)	1735(15)	-18(8)	105(9)
C <sub>4e</sub>	-1410(10)	852(19)	-89(11)	94(11)
C <sub>4f</sub>	-1123(7)	204(15)	390(7)	65(7)
C <sub>4g</sub>	-1533(8)	1444(15)	1523(10)	93(10)
C <sub>4h</sub>	-2063(10)	1579(29)	1450(11)	214(21)
C <sub>4i</sub>	-815(8)	-747(16)	295(8)	87(9)
C <sub>4j</sub>	-1208(11)	-1692(22)	34(10)	141(13)

<sup>a</sup> The numbers in parentheses are the estimated standard deviations in the last significant digit.

<sup>b</sup> Atoms are labeled in agreement with Figure 1.

<sup>c</sup> This is one-third of the trace of the orthogonalized B<sub>ij</sub> tensor.

Table II. Anisotropic Thermal Parameters for Nonhydrogen Atoms in Crystalline  $[\text{Sn}(\text{C}_6\text{H}_3(\text{C}_2\text{H}_5)_2)]_8$ <sup>a,b</sup>

Atom	Anisotropic Thermal Parameters ( $\text{\AA}^2 \times 10$ )					
Type <sup>c</sup>	B <sub>11</sub>	B <sub>22</sub>	B <sub>33</sub>	B <sub>12</sub>	B <sub>13</sub>	B <sub>23</sub>
Sn <sub>1</sub>	40(1)	46(1)	45(1)	-4(1)	17(1)	5(1)
Sn <sub>2</sub>	42(1)	43(1)	46(1)	2(1)	20(1)	-3(1)
Sn <sub>3</sub>	41(1)	42(1)	39(1)	-4(1)	15(1)	-5(1)
Sn <sub>4</sub>	37(1)	39(1)	44(1)	2(1)	8(1)	4(1)
C <sub>1a</sub>	48(8)	78(12)	48(9)	-27(8)	19(7)	14(8)
C <sub>1b</sub>	77(11)	100(15)	69(11)	-40(10)	34(9)	25(10)
C <sub>1c</sub>	76(12)	71(12)	103(14)	-8(9)	36(11)	17(10)
C <sub>1d</sub>	76(12)	105(17)	129(17)	-27(11)	59(12)	21(14)
C <sub>1e</sub>	65(11)	110(19)	151(19)	3(12)	58(12)	15(15)
C <sub>1f</sub>	53(11)	90(14)	106(15)	-5(10)	40(11)	10(12)
C <sub>1g</sub>	78(14)	78(17)	137(23)	-18(14)	47(15)	38(18)
C <sub>1h</sub>	102(17)	75(13)	173(21)	-1(11)	65(16)	2(13)
C <sub>1i</sub>	47(9)	120(17)	182(21)	-7(10)	53(12)	69(16)
C <sub>1j</sub>	130(19)	75(13)	205(24)	-7(15)	81(18)	-22(16)
C <sub>2a</sub>	47(8)	46(9)	32(7)	18(6)	8(6)	4(6)
C <sub>2b</sub>	80(12)	84(15)	58(9)	18(11)	30(9)	5(10)
C <sub>2c</sub>	133(19)	141(21)	85(14)	37(16)	72(14)	-11(14)
C <sub>2d</sub>	134(18)	138(20)	102(15)	41(16)	88(14)	-7(15)
C <sub>2e</sub>	64(12)	117(19)	82(13)	36(12)	17(10)	-15(14)
C <sub>2f</sub>	66(10)	62(11)	74(10)	-1(8)	29(8)	-24(9)
C <sub>2g</sub>	151(20)	156(20)	80(13)	60(16)	85(14)	23(13)
C <sub>2h</sub>	157(24)	284(32)	82(17)	116(22)	26(16)	57(19)

Table II. (continued)

Atom	Anisotropic Thermal Parameters ( $\text{\AA}^2 \times 10$ )					
Type <sup>c</sup>	B <sub>11</sub>	B <sub>22</sub>	B <sub>33</sub>	B <sub>12</sub>	B <sub>13</sub>	B <sub>23</sub>
C <sub>2i</sub>	171(21)	114(18)	59(12)	105(17)	39(13)	21(12)
C <sub>2j</sub>	501(55)	88(21)	163(24)	-51(29)	207(31)	-5(19)
C <sub>3a</sub>	49(8)	44(8)	34(6)	-9(6)	13(6)	-12(6)
C <sub>3b</sub>	53(10)	72(12)	62(9)	-28(9)	6(8)	-20(8)
C <sub>3c</sub>	85(14)	92(16)	81(15)	-23(13)	9(11)	-17(12)
C <sub>3d</sub>	76(16)	141(19)	67(12)	-62(16)	24(11)	-39(13)
C <sub>3e</sub>	138(17)	70(12)	85(13)	-59(13)	63(13)	-54(11)
C <sub>3f</sub>	60(10)	80(12)	69(11)	-1(9)	30(8)	-11(10)
C <sub>3g</sub>	52(10)	92(13)	115(15)	-13(9)	35(10)	-25(12)
C <sub>3h</sub>	126(17)	96(16)	111(16)	42(13)	3(13)	19(13)
C <sub>3i</sub>	130(19)	126(21)	136(18)	-61(15)	67(16)	-113(17)
C <sub>3j</sub>	88(16)	92(18)	356(46)	33(14)	59(22)	76(22)
C <sub>4a</sub>	40(7)	56(10)	54(9)	-15(6)	-1(6)	16(7)
C <sub>4b</sub>	36(8)	43(9)	100(13)	6(7)	1(8)	6(9)
C <sub>4c</sub>	36(8)	66(13)	133(18)	-6(8)	12(10)	39(13)
C <sub>4d</sub>	93(13)	103(15)	88(12)	-23(13)	12(10)	53(12)
C <sub>4e</sub>	87(16)	116(18)	60(13)	-26(14)	16(12)	26(14)
C <sub>4f</sub>	57(9)	83(12)	37(8)	-3(8)	4(7)	16(8)
C <sub>4g</sub>	93(13)	69(14)	93(15)	39(10)	21(11)	-4(11)
C <sub>4h</sub>	113(16)	432(52)	122(19)	92(26)	73(15)	27(29)
C <sub>4i</sub>	85(13)	112(16)	57(10)	6(12)	26(9)	10(10)
C <sub>4j</sub>	124(19)	163(24)	79(13)	11(20)	-5(12)	18(17)

<sup>a</sup> The numbers in parentheses are the estimated standard deviations in the last significant digit.

<sup>b</sup> The form of the anisotropic thermal parameter is given in reference 8 on page 6 of the structure report.

<sup>c</sup> Atoms are labeled in agreement with Figure 1.

Table III. Atomic Coordinates for Hydrogen Atoms in  
Crystalline  $[\text{Sn}(\text{C}_6\text{H}_3(\text{C}_2\text{H}_5)_2)]_8^a$

Atom Type <sup>b</sup>	Fractional Coordinates		
	$10^4x$	$10^4y$	$10^4z$
H <sub>1c</sub>	1005	2708	1282
H <sub>1d</sub>	1905	2279	1572
H <sub>1e</sub>	2258	690	2018
H <sub>1ga</sub>	-35	1102	1241
H <sub>1gb</sub>	81	2184	1054
H <sub>1ia</sub>	2180	-629	2687
H <sub>1ib</sub>	1606	-1133	2508
H <sub>2c</sub>	1038	-3871	461
H <sub>2d</sub>	1552	-5281	957
H <sub>2e</sub>	1752	-5624	1932
H <sub>2ga</sub>	667	-2021	916
H <sub>2gb</sub>	142	-2616	847
H <sub>2ia</sub>	1093	-4431	2707
H <sub>2ib</sub>	1700	-4715	2862
H <sub>3c</sub>	-2596	-4119	572
H <sub>3d</sub>	-2437	-5352	43
H <sub>3e</sub>	-1568	-5653	147
H <sub>3ga</sub>	-1687	-2409	1596
H <sub>3gb</sub>	-2224	-3023	1459
H <sub>3ia</sub>	-417	-4084	932
H <sub>3ib</sub>	-672	-4874	412
H <sub>4c</sub>	-1922	2430	544
H <sub>4d</sub>	-1837	2223	-334

Table III. (continued)

Atom	Fractional Coordinates		
Type <sup>b</sup>	10 <sup>4</sup> x	10 <sup>4</sup> y	10 <sup>4</sup> z
H <sub>4e</sub>	-1425	687	-467
H <sub>4ga</sub>	-1343	2073	1682
H <sub>4gb</sub>	-1361	900	1799
H <sub>4ia</sub>	-518	-931	667
H <sub>4ib</sub>	-672	-545	24

<sup>a</sup> Since of the 8 terminal methyl groups did not give chemically reasonable C-C-H angles when refined as rigid rotors, the methyl hydrogens were omitted from the structure factor calculations. The remaining hydrogen atoms were included in the structure factor calculations as idealized atoms (assuming sp<sup>2</sup>- or sp<sup>3</sup>-hybridization of the carbon atoms and a C-H bond length of 0.96Å) "riding" on their respective carbon atoms. The isotropic thermal parameter of each hydrogen atom was fixed at 1.2 times the equivalent isotropic thermal parameter of the carbon atom to which it is covalently bonded.

<sup>b</sup> Hydrogen atoms are labeled with the same numerical and literal subscripts as the carbon atoms to which they are covalently bonded with an additional literal subscript (a or b) where necessary to distinguish between hydrogens bonded to the same atom.

Table IV. Bond Lengths Involving Nonhydrogen Atoms in Crystalline  $[\text{Sn}(\text{C}_6\text{H}_3(\text{C}_2\text{H}_5)_2)]_8$ <sup>a</sup>

Type <sup>b</sup>	Length, Å	Type <sup>b</sup>	Length, Å
$\text{Sn}_1\text{-Sn}_2$	2.857(2)	$\text{Sn}_2\text{-Sn}_3$	2.853(2)
$\text{Sn}_1\text{-Sn}_4$	2.864(2)	$\text{Sn}_2\text{-Sn}_3$ , <sup>c</sup>	2.855(2)
$\text{Sn}_1\text{-Sn}_4$ , <sup>c</sup>	2.858(2)	$\text{Sn}_3\text{-Sn}_4$	2.839(2)
$\text{Sn}_1\text{-C}_{1a}$	2.17(2)	$\text{Sn}_3\text{-C}_{3a}$	2.18(1)
$\text{Sn}_2\text{-C}_{2a}$	2.20(2)	$\text{Sn}_4\text{-C}_{4a}$	2.22(2)
$\text{C}_{1a}\text{-C}_{1b}$	1.40(2)	$\text{C}_{3a}\text{-C}_{3b}$	1.40(3)
$\text{C}_{1a}\text{-C}_{1f}$	1.42(3)	$\text{C}_{3a}\text{-C}_{3f}$	1.34(3)
$\text{C}_{1b}\text{-C}_{1c}$	1.42(3)	$\text{C}_{3b}\text{-C}_{3c}$	1.37(3)
$\text{C}_{1c}\text{-C}_{1d}$	1.33(3)	$\text{C}_{3c}\text{-C}_{3d}$	1.32(4)
$\text{C}_{1d}\text{-C}_{1e}$	1.40(3)	$\text{C}_{3d}\text{-C}_{3e}$	1.33(4)
$\text{C}_{1e}\text{-C}_{1f}$	1.40(4)	$\text{C}_{3e}\text{-C}_{3f}$	1.44(3)
$\text{C}_{2a}\text{-C}_{2b}$	1.34(3)	$\text{C}_{4a}\text{-C}_{4b}$	1.40(3)
$\text{C}_{2a}\text{-C}_{2f}$	1.42(2)	$\text{C}_{4a}\text{-C}_{4f}$	1.40(3)
$\text{C}_{2b}\text{-C}_{2c}$	1.40(4)	$\text{C}_{4b}\text{-C}_{4c}$	1.37(3)
$\text{C}_{2c}\text{-C}_{2d}$	1.36(3)	$\text{C}_{4c}\text{-C}_{4d}$	1.39(4)
$\text{C}_{2d}\text{-C}_{2e}$	1.38(4)	$\text{C}_{4d}\text{-C}_{4e}$	1.43(4)
$\text{C}_{2e}\text{-C}_{2f}$	1.40(4)	$\text{C}_{4e}\text{-C}_{4f}$	1.40(3)
$\text{C}_{1b}\text{-C}_{1g}$	1.60(3)	$\text{C}_{3b}\text{-C}_{3g}$	1.56(3)
$\text{C}_{1f}\text{-C}_{1i}$	1.54(3)	$\text{C}_{3f}\text{-C}_{3i}$	1.56(3)
$\text{C}_{2b}\text{-C}_{2g}$	1.56(3)	$\text{C}_{4b}\text{-C}_{4g}$	1.50(4)
$\text{C}_{2f}\text{-C}_{2i}$	1.52(3)	$\text{C}_{4f}\text{-C}_{4i}$	1.58(3)



Table IV. (continued)

Type <sup>b</sup>	Length, Å	Type <sup>b</sup>	Length, Å
C <sub>1g</sub> -C <sub>1h</sub>	1.52(4)	C <sub>3g</sub> -C <sub>3h</sub>	1.49(3)
C <sub>1i</sub> -C <sub>1j</sub>	1.53(4)	C <sub>3i</sub> -C <sub>3j</sub>	1.40(4)
C <sub>2g</sub> -C <sub>2h</sub>	1.40(3)	C <sub>4g</sub> -C <sub>4h</sub>	1.39(4)
C <sub>2i</sub> -C <sub>2j</sub>	1.18(4)	C <sub>4i</sub> -C <sub>4j</sub>	1.58(3)

- <sup>a</sup> The numbers in parentheses are the estimated standard deviations in the last significant digit.
- <sup>b</sup> Atoms are labeled in agreement with Figure 1.
- <sup>c</sup> Atoms labeled with a prime (') are related to nonprimed atoms by the crystallographic C<sub>2</sub>-axis at 0,y,1/4 in the unit cell.

Table V. Bond Angles Involving Nonhydrogen Atoms in Crystalline  $[\text{Sn}(\text{C}_6\text{H}_3(\text{C}_2\text{H}_5)_2)]_8$ <sup>a</sup>

Type <sup>b</sup>	Angle, deg.	Type <sup>b</sup>	Angle, deg.
$\text{Sn}_2\text{Sn}_1\text{Sn}_4$	90.6(1)	$\text{Sn}_2\text{Sn}_1\text{C}_{1a}$	128.6(5)
$\text{Sn}_2\text{Sn}_1\text{Sn}_4,^c$	89.8(1)	$\text{Sn}_4\text{Sn}_1\text{C}_{1a}$	129.0(4)
$\text{Sn}_4\text{Sn}_1\text{Sn}_4,^c$	89.9(1)	$\text{Sn}_4, \text{Sn}_1\text{C}_{1a}^c$	117.3(4)
$\text{Sn}_1\text{Sn}_2\text{Sn}_3$	89.1(1)	$\text{Sn}_1\text{Sn}_2\text{C}_{2a}$	123.3(4)
$\text{Sn}_1\text{Sn}_2\text{Sn}_3,^c$	89.8(1)	$\text{Sn}_3\text{Sn}_2\text{C}_{2a}$	122.1(4)
$\text{Sn}_3\text{Sn}_2\text{Sn}_3,^c$	90.2(1)	$\text{Sn}_3, \text{Sn}_2\text{C}_{2a}^c$	130.8(4)
$\text{Sn}_2\text{Sn}_3\text{Sn}_4$	91.1(1)	$\text{Sn}_2\text{Sn}_3\text{C}_{3a}$	131.8(5)
$\text{Sn}_2\text{Sn}_3\text{Sn}_2,^c$	89.8(1)	$\text{Sn}_4\text{Sn}_3\text{C}_{3a}$	124.7(4)
$\text{Sn}_4\text{Sn}_3\text{Sn}_2,^c$	90.3(1)	$\text{Sn}_2, \text{Sn}_3\text{C}_{3a}^c$	117.7(5)
$\text{Sn}_1\text{Sn}_4\text{Sn}_3$	89.2(1)	$\text{Sn}_1\text{Sn}_4\text{C}_{4a}$	117.4(5)
$\text{Sn}_1\text{Sn}_4\text{Sn}_1,^c$	90.1(1)	$\text{Sn}_3\text{Sn}_4\text{C}_{4a}$	125.0(4)
$\text{Sn}_3\text{Sn}_4\text{Sn}_1,^c$	90.1(1)	$\text{Sn}_1, \text{Sn}_4\text{C}_{4a}^c$	133.0(5)
$\text{Sn}_1\text{C}_{1a}\text{C}_{1b}$	122(1)	$\text{Sn}_3\text{C}_{3a}\text{C}_{3b}$	117(1)
$\text{Sn}_1\text{C}_{1a}\text{C}_{1f}$	119(1)	$\text{Sn}_3\text{C}_{3a}\text{C}_{3f}$	124(1)
$\text{C}_{1b}\text{C}_{1a}\text{C}_{1f}$	118(2)	$\text{C}_{3b}\text{C}_{3a}\text{C}_{3f}$	119(1)
$\text{C}_{1a}\text{C}_{1b}\text{C}_{1c}$	122(2)	$\text{C}_{3a}\text{C}_{3b}\text{C}_{3c}$	118(2)
$\text{C}_{1a}\text{C}_{1b}\text{C}_{1g}$	121(2)	$\text{C}_{3a}\text{C}_{3b}\text{C}_{3g}$	126(1)
$\text{C}_{1c}\text{C}_{1b}\text{C}_{1g}$	116(2)	$\text{C}_{3c}\text{C}_{3b}\text{C}_{3g}$	116(2)
$\text{C}_{1b}\text{C}_{1c}\text{C}_{1d}$	118(2)	$\text{C}_{3b}\text{C}_{3c}\text{C}_{3d}$	123(2)
$\text{C}_{1c}\text{C}_{1d}\text{C}_{1e}$	122(2)	$\text{C}_{3c}\text{C}_{3d}\text{C}_{3e}$	121(2)
$\text{C}_{1d}\text{C}_{1e}\text{C}_{1f}$	121(2)	$\text{C}_{3d}\text{C}_{3e}\text{C}_{3f}$	118(2)
$\text{C}_{1a}\text{C}_{1f}\text{C}_{1e}$	118(2)	$\text{C}_{3a}\text{C}_{3f}\text{C}_{3e}$	121(2)

Table V. (continued)

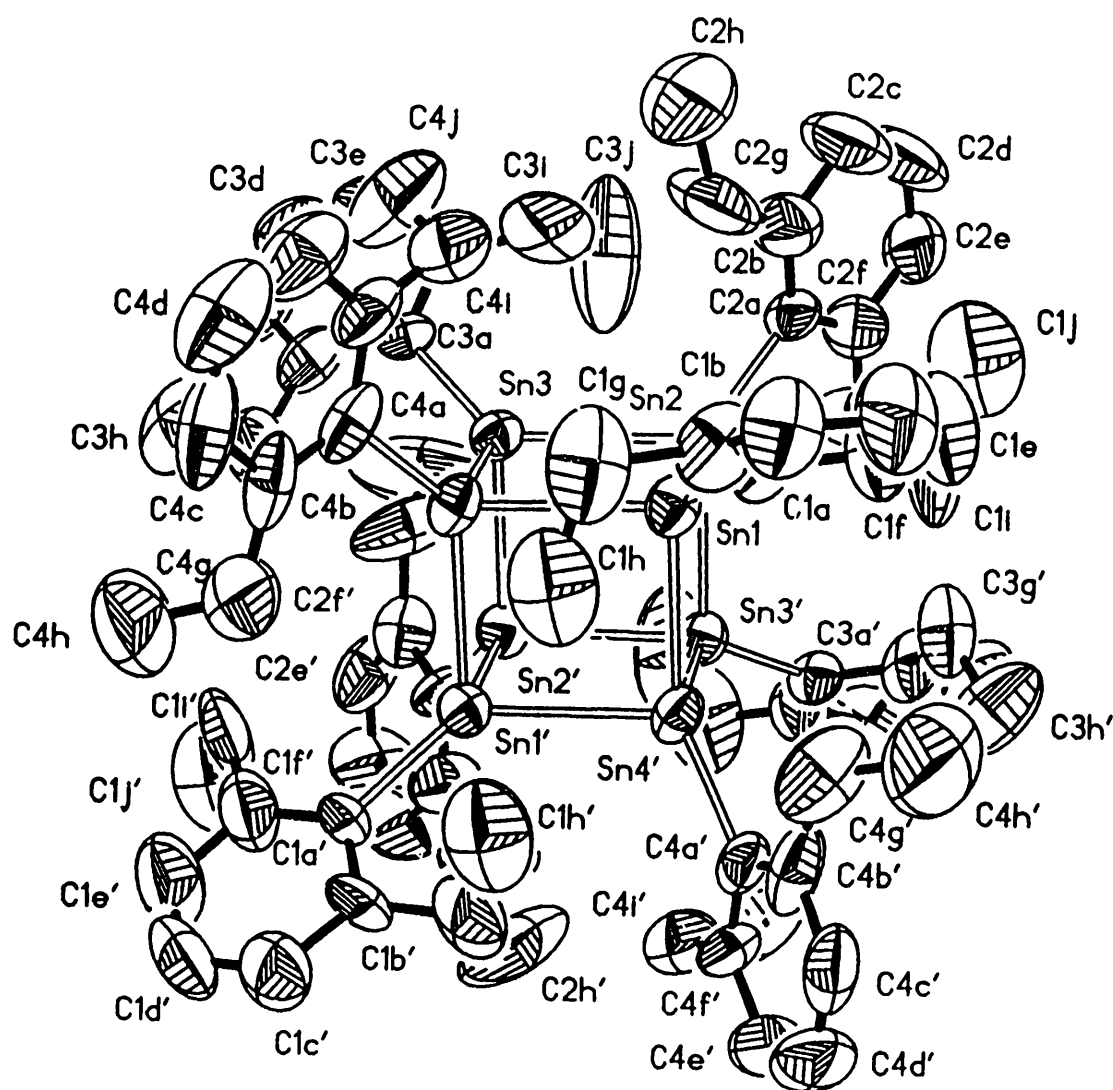
Type <sup>b</sup>	Angle, deg.	Type <sup>b</sup>	Angle, deg.
C <sub>1a</sub> C <sub>1f</sub> C <sub>1i</sub>	124(2)	C <sub>3a</sub> C <sub>3f</sub> C <sub>3i</sub>	122(2)
C <sub>1e</sub> C <sub>1f</sub> C <sub>1i</sub>	117(2)	C <sub>3e</sub> C <sub>3f</sub> C <sub>3i</sub>	116(2)
Sn <sub>2</sub> C <sub>2a</sub> C <sub>2b</sub>	121(1)	Sn <sub>4</sub> C <sub>4a</sub> C <sub>4b</sub>	120(1)
Sn <sub>2</sub> C <sub>2a</sub> C <sub>2f</sub>	119(1)	Sn <sub>4</sub> C <sub>4a</sub> C <sub>4f</sub>	119(1)
C <sub>2b</sub> C <sub>2a</sub> C <sub>2f</sub>	120(2)	C <sub>4b</sub> C <sub>4a</sub> C <sub>4f</sub>	121(2)
C <sub>2a</sub> C <sub>2b</sub> C <sub>2c</sub>	124(2)	C <sub>4a</sub> C <sub>4b</sub> C <sub>4c</sub>	119(2)
C <sub>2a</sub> C <sub>2b</sub> C <sub>2g</sub>	123(2)	C <sub>4a</sub> C <sub>4b</sub> C <sub>4g</sub>	126(2)
C <sub>2c</sub> C <sub>2b</sub> C <sub>2g</sub>	113(2)	C <sub>4c</sub> C <sub>4b</sub> C <sub>4g</sub>	115(2)
C <sub>2b</sub> C <sub>2c</sub> C <sub>2d</sub>	115(2)	C <sub>4b</sub> C <sub>4c</sub> C <sub>4d</sub>	122(2)
C <sub>2c</sub> C <sub>2d</sub> C <sub>2e</sub>	123(3)	C <sub>4c</sub> C <sub>4d</sub> C <sub>4e</sub>	118(2)
C <sub>2d</sub> C <sub>2e</sub> C <sub>2f</sub>	120(2)	C <sub>4d</sub> C <sub>4e</sub> C <sub>4f</sub>	120(2)
C <sub>2a</sub> C <sub>2f</sub> C <sub>2e</sub>	117(2)	C <sub>4a</sub> C <sub>4f</sub> C <sub>4e</sub>	118(2)
C <sub>2a</sub> C <sub>2f</sub> C <sub>2i</sub>	124(2)	C <sub>4a</sub> C <sub>4f</sub> C <sub>4i</sub>	123(2)
C <sub>2e</sub> C <sub>2f</sub> C <sub>2i</sub>	120(2)	C <sub>4e</sub> C <sub>4f</sub> C <sub>4i</sub>	119(2)
C <sub>1b</sub> C <sub>1g</sub> C <sub>1h</sub>	113(2)	C <sub>3b</sub> C <sub>3g</sub> C <sub>3h</sub>	114(2)
C <sub>1f</sub> C <sub>1i</sub> C <sub>1j</sub>	117(2)	C <sub>3f</sub> C <sub>3i</sub> C <sub>3j</sub>	121(3)
C <sub>2b</sub> C <sub>2g</sub> C <sub>2h</sub>	122(2)	C <sub>4b</sub> C <sub>4g</sub> C <sub>4h</sub>	118(2)
C <sub>2f</sub> C <sub>2i</sub> C <sub>2j</sub>	131(3)	C <sub>4f</sub> C <sub>4i</sub> C <sub>4j</sub>	112(2)

<sup>a</sup> The numbers in parentheses are the estimated standard deviations in the last significant digit.

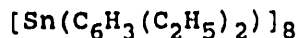
<sup>b</sup> Atoms are labeled in agreement with Figure 1.

<sup>c</sup> Atoms labeled with a prime (') are related to nonprimed atoms by the crystallographic C<sub>2</sub>-axis at 0,y,1/4 in the unit cell.

Figure 2. Molecular structure of 1 with all nonhydrogen atoms represented by thermal vibration ellipsoids drawn to encompass 50% of their electron density. Atoms labeled with a prime (') are related to nonprimed atoms by the crystallographic  $C_2$ -axis at  $0, y, 1/4$  in the unit cell. Hydrogen atoms have been omitted for purposes of clarity.



## Structure Factor Amplitude Tables for



2221 Reflections

Entries for each reflection include:

Miller Indices,  $F_o \times 10$ ,  $F_c \times 10$ 

H	K	L	FOBS	FCAL	H	K	L	FOBS	FCAL	H	K	L	FOBS	FCAL	H	K	L	FOBS	FCAL
2	0	0	9345	9901	4	6	0	964	937	1	1	1	7038	7479	-11	5	1	5400	5411
4	0	0	3276	3565	6	6	0	3463	3471	3	1	1	3525	3369	-9	5	1	8084	8140
6	0	0	5686	5464	8	6	0	4349	4297	5	1	1	3722	3571	-7	5	1	5708	5803
8	0	0	106131	10231	10	6	0	2971	2973	7	1	1	6143	5875	-3	5	1	4706	4703
10	0	0	7941	7739	12	6	0	1082	1069	9	1	1	4774	4684	-1	5	1	8240	8194
12	0	0	2709	2721	14	6	0	1190	1190	11	1	1	2778	2709	1	5	1	6829	6669
14	0	0	2431	2354	16	6	0	2081	2080	15	1	1	2140	2134	3	5	1	2679	2653
16	0	0	4514	4524	18	6	0	1353	1322	17	1	1	1469	1441	5	5	1	2544	2438
18	0	0	3652	3715	24	6	0	544	573	-18	2	1	734	821	7	5	1	5044	4951
20	0	0	1358	1317	11	7	0	686	567	-16	2	1	1185	1204	9	5	1	4311	4323
24	0	0	1143	1163	0	8	0	2658	2747	-14	2	1	731	754	11	5	1	1898	1790
26	0	0	732	859	2	8	0	2036	1998	-10	2	1	2233	2175	13	5	1	856	898
1	1	0	5202	5118	6	8	0	1343	1355	-8	2	1	3462	3344	15	5	1	1821	1724
3	1	0	2034	2181	8	8	0	1977	1951	-6	2	1	952	837	17	5	1	1651	1660
5	1	0	676	722	10	8	0	1540	1516	-4	2	1	4513	4540	8	6	1	857	759
7	1	0	4020	3845	16	8	0	1068	1046	-2	2	1	1022	1008	9	7	1	644	475
9	1	0	3983	4112	18	8	0	901	939	0	2	1	1086	1250	-20	8	1	903	945
11	1	0	1172	1083	1	9	0	5849	5768	2	2	1	1429	1510	-18	8	1	1627	1635
15	1	0	1252	1287	3	9	0	2496	2503	4	2	1	1034	962	-16	8	1	1844	1853
17	1	0	1697	1702	5	9	0	1297	1277	6	2	1	1499	1399	-12	8	1	1581	1655
19	1	0	954	1073	7	9	0	4398	4385	8	2	1	1036	977	-10	8	1	2834	2941
0	2	0	866	899	9	9	0	4628	4538	10	2	1	1065	983	-8	8	1	3359	3316
2	2	0	1585	1703	11	9	0	2495	2473	12	2	1	783	718	-6	8	1	1508	1508
4	2	0	3633	3365	15	9	0	1887	1883	-7	3	1	686	595	-4	8	1	1448	1478
8	2	0	2091	2070	17	9	0	2162	2194	-5	3	1	885	863	-2	8	1	3153	3130
16	2	0	754	649	19	9	0	1284	1301	-1	3	1	138	119	0	8	1	3581	3600
1	3	0	3516	3574	0	10	0	2131	2138	1	3	1	568	538	2	8	1	2481	2505
3	3	0	5002	4754	2	10	0	1539	1548	5	3	1	1437	1381	6	8	1	2176	2083
5	3	0	3123	2957	6	10	0	1257	1272	-26	4	1	1240	1284	8	8	1	2803	2683
7	3	0	5087	5083	8	10	0	1606	1571	-24	4	1	1062	1159	10	8	1	1600	1589
9	3	0	3781	3647	10	10	0	964	1007	-20	4	1	1600	1691	16	8	1	881	811
11	3	0	1821	1776	16	10	0	731	773	-18	4	1	3344	3374	-18	10	1	1732	1722
15	3	0	1514	1490	7	11	0	597	574	-16	4	1	3685	3818	-16	10	1	1841	1795
17	3	0	1925	1897	9	11	0	574	623	-14	4	1	1349	1439	-12	10	1	1227	1195
19	3	0	1164	1147	0	12	0	1337	1359	-12	4	1	2336	2469	-10	10	1	2782	2748
0	4	0	5746	5581	2	12	0	1112	1057	-10	4	1	7748	7876	-8	10	1	3125	3151
2	4	0	4686	4347	8	12	0	785	725	-8	4	1	7639	7577	-6	10	1	1835	1817
4	4	0	897	853	10	12	0	754	806	-6	4	1	2672	2649	-4	10	1	755	636
6	4	0	2349	2312	1	13	0	1016	1029	-4	4	1	2127	2089	-2	10	1	3118	3154
8	4	0	3598	3462	7	13	0	677	745	-2	4	1	8316	8145	0	10	1	4010	4031
10	4	0	3277	3192	9	13	0	795	780	0	4	1	9752	9556	2	10	1	2075	2104
12	4	0	1493	1491	0	14	0	1435	1331	2	4	1	6476	6273	6	10	1	2016	1944
14	4	0	781	806	2	14	0	947	952	4	4	1	967	882	8	10	1	2293	2358
16	4	0	1618	1747	-27	1	1	936	967	6	4	1	4482	4336	10	10	1	1703	1702
18	4	0	1797	1788	-25	1	1	1284	1316	8	4	1	6760	6431	14	10	1	884	856
1	5	0	4805	4803	-21	1	1	847	866	10	4	1	2984	2859	16	10	1	977	937
3	5	0	2277	2253	-19	1	1	2758	2739	12	4	1	634	714	-17	11	1	669	634
5	5	0	750	798	-17	1	1	4052	4120	14	4	1	1156	1318	-9	11	1	1039	956
7	5	0	3966	3918	-15	1	1	2875	2854	16	4	1	1994	1894	-7	11	1	782	821
9	5	0	4639	4542	-13	1	1	918	1016	18	4	1	1363	1321	-1	11	1	1069	1222
11	5	0	2516	2504	-11	1	1	4571	4618	-25	5	1	1216	1230	1	11	1	929	858
15	5	0	1918	2000	-9	1	1	8025	7827	-23	5	1	794	791	7	11	1	795	767
17	5	0	1358	1385	-7	1	1	9020	8817	-21	5	1	715	602	-11	13	1	1169	1280
19	5	0	1019	1062	-5	1	1	785	776	-19	5	1	2374	2517	-9	13	1	1907	1880
0	6	0	4634	4801	-3	1	1	4423	4494	-17	5	1	3661	3680	-7	13	1	1561	1494
2	6	0	4302	4349	-1	1	1	8365	8821	-15	5	1	3258	3351	-3	13	1	1187	1232

H	K	L	FOBS	FCAL	H	K	L	FOBS	FCAL	H	K	L	FOBS	FCAL	H	K	L	FOBS	FCAL
-1	13	1	2136	2113	8	2	2	700	578	0	6	2	3864	3828	-25	1	3	1610	1623
1	13	1	1703	1755	-27	3	2	839	914	2	6	2	1202	1264	-21	1	3	1816	1711
3	13	1	701	576	-25	3	2	1027	1063	4	6	2	731	761	-19	1	3	3938	3880
7	13	1	1309	1321	-21	3	2	842	904	6	6	2	1707	1729	-17	1	3	3764	3769
9	13	1	1357	1257	-19	3	2	2613	2594	8	6	2	2169	2188	-15	1	3	1518	1498
-6	14	1	820	733	-17	3	2	2905	2939	-20	8	2	755	831	-13	1	3	1210	1180
-4	14	1	659	600	-15	3	2	694	732	-18	8	2	1344	1304	-11	1	3	4800	4600
-2	14	1	1378	1474	-11	3	2	2876	2976	-16	8	2	1124	1108	-9	1	3	5692	5725
0	14	1	1749	1620	-9	3	2	4901	5006	-12	8	2	1286	1258	-7	1	3	1142	1128
2	14	1	898	1031	-7	3	2	3323	3386	-10	8	2	1998	2026	-5	1	3	778	803
-26	0	2	2511	2423	-3	3	2	3131	2951	-8	8	2	2188	2199	-3	1	3	3817	3874
-24	0	2	2068	2086	-1	3	2	4364	4424	-4	8	2	1128	1120	-1	1	3	4329	4570
-20	0	2	3969	3967	1	3	2	3260	3161	-2	8	2	1725	1808	1	1	3	1167	1049
-18	0	2	5891	5887	7	3	2	2742	2713	0	8	2	1891	1916	5	1	3	737	720
-16	0	2	5255	5370	9	3	2	2309	2248	2	8	2	1131	1123	7	1	3	1319	1310
-12	0	2	5696	5688	11	3	2	932	980	6	8	2	902	895	9	1	3	692	729
-10	0	2	9050	8773	-26	4	2	943	821	10	8	2	667	412	15	1	3	842	837
-8	0	2	10902	10419	-24	4	2	742	780	-21	9	2	1011	1094	17	1	3	1167	1143
-6	0	2	2360	2394	-20	4	2	1380	1466	-19	9	2	2457	2593	19	1	3	836	691
-4	0	2	2058	2140	-18	4	2	2288	2350	-17	9	2	2968	2936	23	1	3	856	835
-2	0	2	94791	10139	-16	4	2	1981	2006	-15	9	2	1661	1695	25	1	3	895	923
0	0	2	8817	9274	-12	4	2	1191	1329	-13	9	2	1028	1101	-18	2	3	1022	1130
2	0	2	4952	5116	-10	4	2	4739	4770	-11	9	2	3775	3706	-16	2	3	789	933
6	0	2	5210	4970	-8	4	2	4047	4019	-9	9	2	4856	4804	-10	2	3	1435	1368
8	0	2	5359	5190	-4	4	2	1856	1813	-7	9	2	3345	3504	-8	2	3	1059	1130
10	0	2	2855	2724	-2	4	2	3738	3600	-3	9	2	3296	3323	-2	2	3	1692	1720
14	0	2	1515	1506	0	4	2	3523	3521	-1	9	2	4399	4498	0	2	3	4019	3971
16	0	2	738	713	2	4	2	2038	2008	1	9	2	3334	3281	2	2	3	1327	1343
-27	1	2	686	745	4	4	2	2126	2050	3	9	2	830	808	4	2	3	2008	1891
-25	1	2	951	1023	6	4	2	2492	2401	5	9	2	1799	1702	10	2	3	784	679
-21	1	2	1069	852	10	4	2	644	811	7	9	2	2434	2366	14	2	3	761	666
-19	1	2	1955	1869	-25	5	2	955	1030	9	9	2	1558	1583	-1	3	3	787	877
-17	1	2	2321	2305	-21	5	2	918	1003	-20	10	2	617	617	1	3	3	588	606
-15	1	2	1613	1581	-19	5	2	1861	1918	-18	10	2	977	1046	3	3	3	933	933
-13	1	2	988	951	-17	5	2	2604	2762	-16	10	2	877	836	5	3	3	1465	1419
-11	1	2	2901	2994	-15	5	2	1460	1629	-12	10	2	763	734	7	3	3	676	587
-9	1	2	4191	4115	-13	5	2	1021	1086	-10	10	2	1326	1366	-26	4	3	1819	1861
-7	1	2	5784	5544	-11	5	2	2993	2969	-8	10	2	1349	1321	-24	4	3	1227	1266
-5	1	2	1294	1228	-9	5	2	4149	4203	-2	10	2	1480	1500	-22	4	3	764	789
-3	1	2	3297	3582	-7	5	2	2855	2915	0	10	2	1414	1389	-20	4	3	2685	2688
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5	1	2	1436	1460	1	5	2	3125	3066	-17	11	2	638	438	-12	4	3	3863	3974
7	1	2	2115	1950	5	5	2	1466	1462	-1	11	2	815	511	-10	4	3	4999	5072
9	1	2	1821	1788	7	5	2	2413	2360	-12	12	2	668	585	-8	4	3	4924	4847
-16	2	2	809	758	9	5	2	1415	1379	-10	12	2	753	874	-6	4	3	2538	2516
-12	2	2	1086	1054	-24	6	2	1053	998	-8	12	2	811	687	-4	4	3	2209	2177
-10	2	2	1082	1041	-20	6	2	1397	1419	-2	12	2	922	985	-2	4	3	4672	4632
-8	2	2	851	809	-18	6	2	2527	2591	0	12	2	966	975	0	4	3	3935	3846
-6	2	2	1811	1834	-16	6	2	2554	2686	-11	13	2	711	734	2	4	3	838	890
-4	2	2	1147	1194	-12	6	2	1889	1956	-9	13	2	839	837	6	4	3	1785	1687
-2	2	2	815	771	-10	6	2	3608	3607	-1	13	2	862	876	16	4	3	1117	1140
0	2	2	636	669	-8	6	2	3910	4074	-2	14	2	887	856	24	4	3	1018	1082
2	2	2	1089	963	-6	6	2	1280	1358	0	14	2	883	947	-25	5	3	1660	1658
4	2	2	2181	2218	-4	6	2	1681	1705	2	14	2	650	538	-21	5	3	1924	1885
6	2	2	975	1018	-2	6	2	3549	3611	-27	1	3	1608	1647	-19	5	3	2900	2935

H	K	L	FOBS	FCAL	H	K	L	FOBS	FCAL	H	K	L	FOBS	FCAL	H	K	L	FOBS	FCAL
-17	5	3	3699	3793	-14	0	4	1161	1189	17	3	4	1437	1509	14	8	4	745	535
-15	5	3	1808	1758	-12	0	4	4527	4544	19	3	4	800	627	16	8	4	855	903
-13	5	3	2153	2133	-10	0	4	5904	5648	23	3	4	764	741	-21	9	4	1368	1438
-11	5	3	4466	4446	-8	0	4	3540	3449	-26	4	4	981	951	-19	9	4	2243	2304
-9	5	3	5244	5385	-4	0	4	3084	3208	-20	4	4	831	911	-17	9	4	2128	2121
-7	5	3	2901	2934	-2	0	4	3052	3139	-18	4	4	1881	1887	-13	9	4	1409	1414
-3	5	3	3490	3598	0	0	4	562	641	-16	4	4	1076	1111	-11	9	4	2263	2211
-1	5	3	4365	4328	2	0	4	3324	3141	-12	4	4	1386	1407	-9	9	4	2071	2069
1	5	3	1589	1536	4	0	4	727	687	-10	4	4	2455	2427	-7	9	4	864	953
5	5	3	1011	1007	6	0	4	2327	2332	-8	4	4	1266	1264	-3	9	4	1105	1107
15	5	3	861	1015	8	0	4	2227	2246	-6	4	4	771	831	7	9	4	1234	1205
17	5	3	982	953	10	0	4	1694	1684	-4	4	4	694	732	9	9	4	1017	1015
19	5	3	664	679	14	0	4	2691	2720	-2	4	4	591	637	15	9	4	1667	1601
23	5	3	644	830	16	0	4	3675	3642	0	4	4	1203	1167	17	9	4	1712	1678
-10	6	3	880	796	18	0	4	1984	1998	4	4	4	562	530	-20	10	4	683	815
-2	6	3	741	655	22	0	4	1496	1522	8	4	4	1346	1301	-18	10	4	710	807
16	6	3	198	164	24	0	4	2168	2140	10	4	4	883	962	-12	10	4	966	913
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